COMPUTATION AND MEASUREMENTS OF MASS TRANSFER AND DISPERSION COEFFICIENTS IN FLUIDIZED BEDS

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Thursday, April 23, 2009

PROJECT PUBLICATIONS

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DISPERSION COEFFICIENTS

- Jiradilok, V., D. Gidaspow, and R.W. Breault, "Computation of gas of solids dispersion coefficients in turbulent risers and bubbling beds," Chemical Engineering Science 62 (2007) 3397-3409
- Jiradilok, V., D. Gidaspow, R.W. Breault, L.J. Shadle, C. Gunther, and S. Shi, "Computation of turbulence and dispersion of cork in the NETL riser", Chemical Engineering Science 63 (2008) 2135-2148

MASS TRANSFER COEFFICIENTS

- Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, "Kinetic theory based computation of PSRI riser- Part I: Estimate of mass transfer coefficient", Chemical Engineering Science, 64 (2009a) 1195-1211
- Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, "Kinetic theory based computation of PSRI riser- Part II: Computation of mass transfer coefficient with chemical reaction", Chemical Engineering Science, 64 (2009b) 1212-1222
- Kashyap, M. and Gidaspow, D, "Measurement of mass transfer coefficients in a bubbling bed with ozone decomposition", Paper in preparation

IMPROVED FUTUREGEN CONCEPT

- Gidaspow, D. and V. Jiradilok, "Nanoparticle gasifier fuel cell for sustainable energy future," Journal of Power Sources 166 (2007a) 400-410
- Gidaspow, D. and V. Jiradilok, "Efficient Coal Gasifier-Fuel Cell with CO2 Sequestration," The Clearwater Coal Conference, The 32nd International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, U.S.A. June 13, 2007b

Kinetic Theory Model

- Continuity Equation for Phase k

$$\frac{\partial(\rho_k \varepsilon_k)}{\partial t} + \nabla \cdot (\rho_k \varepsilon_k v_k) = \dot{m}_k$$

- Momentum Equation for Phase k

$$\frac{\partial(\rho_k \varepsilon_k v_k)}{\partial t} + \nabla \cdot (\rho_k \varepsilon_k v_k v_k) = \varepsilon_k \rho_k \tilde{g} + \nabla \cdot [\tau_k] + \sum_l^N \beta (v_l - v_k) + \dot{m}_k \tilde{v}_k$$

acceleration of phase 'k' = buoyancy + stress + drag force + phase change

- Constitutive Equation for Stress (Above Min. Fluidization)

$$[\tau_k] = [-P_k + \xi_k \nabla v_k][I] + 2\mu_k [S_k]$$

$$[S_k] = \frac{1}{2}\left[\nabla v_k + (\nabla v_k)^T\right] - \frac{1}{3} \nabla \cdot v_k [I]$$

- Solid Phase Stress

  - *Solid-phase Pressure*

$$P_s = \rho_s \varepsilon_s \theta \left[1 + 2(1+e) g_o \varepsilon_s \right]$$

kinetic collision

  - *Solid-phase Bulk Viscosity*

$$\lambda_s = \frac{4}{3} \varepsilon_s^2 \rho_s d_s g_o (1+e) \sqrt{\frac{\theta}{\pi}}$$

  - *Solid-phase Shear Viscosity*

$$\mu_s = \frac{2\mu_{s_{dil}}}{(1+e) g_0} \left[1 + \frac{4}{5}(1+e) g_o \varepsilon_s \right] + \frac{4}{5} \varepsilon_s^2 \rho_s d_s g_o (1+e) \sqrt{\frac{\theta}{\pi}}$$

- Radial distribution function [Bagnold(1954)]

$$g_o = \left[1 - \left(\frac{\varepsilon_s}{\varepsilon_{s,\max}} \right)^{1/3} \right]^{-1}$$

- Solid-phase dilute viscosity

$$\mu_{s_{dil}} = \frac{5\sqrt{\pi}}{96} \rho_p d_p \theta^{1/2}$$

- Fluctuating Energy Equation $(\theta = \frac{1}{3} < C^2 >)$

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s \rho_s \theta) + \nabla \cdot (\varepsilon_s \rho_s v_s \theta)\right] = \overline{\overline{\tau}}_s : \nabla v_s - q - \gamma_s + \beta_A < C_g \cdot C_p > -3\beta_A \theta$$

- Collisional Energy Dissipation

$$\gamma_s = 3(1 - e^2)\varepsilon_s^2 \rho_s g_o \theta \left(\frac{4}{d_s}\sqrt{\frac{\theta}{\pi}} - \nabla \cdot v_s \right)$$

- Conductivity of Fluctuating Energy $(q = -\kappa \nabla \theta)$

$$\kappa = \frac{2}{(1+e)g_0}\left[1 + \frac{6}{5}(1+e)g_o \varepsilon_s\right]^2 \kappa_{dil} + 2\varepsilon_s^2 \rho_s d_s g_o (1+e)\sqrt{\frac{\theta}{\pi}}$$

-Dilute Phase (Eddy Type) Granular Conductivity

$$\kappa_{dil} = \frac{75}{384}\sqrt{\pi \rho_s} d_s \theta^{1/2}$$

- Gas-Solid Drag Coefficients

  - Based on Ergun equation, for $\varepsilon_g < 0.8$

$$\beta = 150\frac{\varepsilon_s^2\mu_g}{\varepsilon_g(d_p\phi_s)^2} + 1.75\frac{\rho_g\varepsilon_s\left|v_g - v_s\right|}{d_p\phi_s}$$

  - Based on single sphere drag, for $\varepsilon_g > 0.8$

$$\beta = \frac{3}{4}C_d\frac{\rho_g\varepsilon_s\varepsilon_g\left|v_g - v_s\right|}{d_p\phi_s}\varepsilon_g^{-2.65}$$

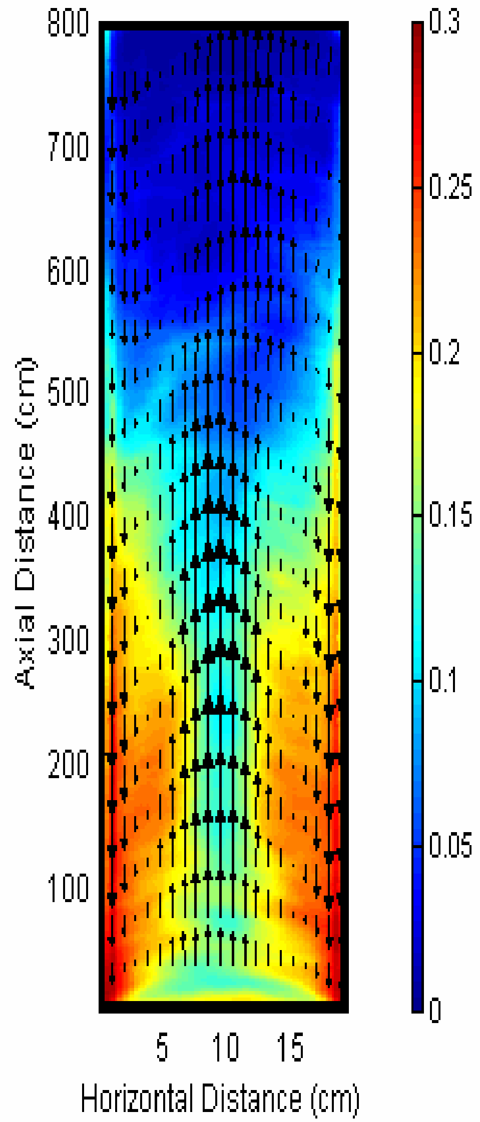
where,

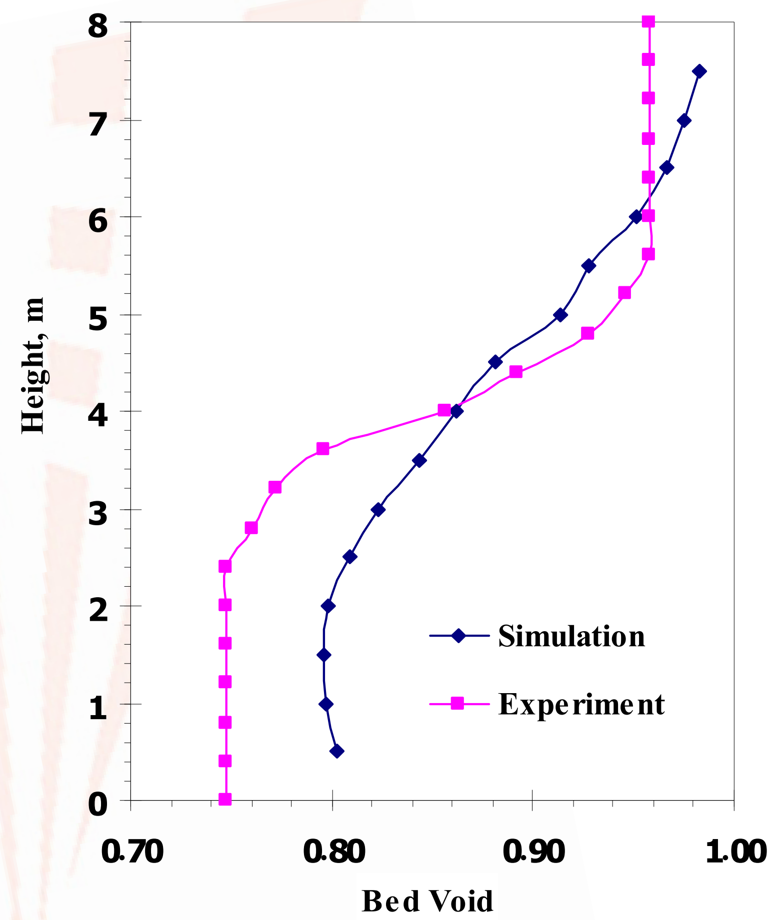
$$C_d = \frac{24}{\mathrm{Re}_p}\left[1 + 0.15\,\mathrm{Re}_p^{0.687}\right] \quad \text{for} \quad \mathrm{Re}_p < 1000$$

$$C_d = 0.44 \qquad \text{for} \quad \mathrm{Re}_p > 1000$$

$$\mathrm{Re}_p = \frac{\varepsilon_g\rho_g d_p\left|v_g - v_s\right|}{\mu_g}$$

Wei et al. (1998) FCC riser

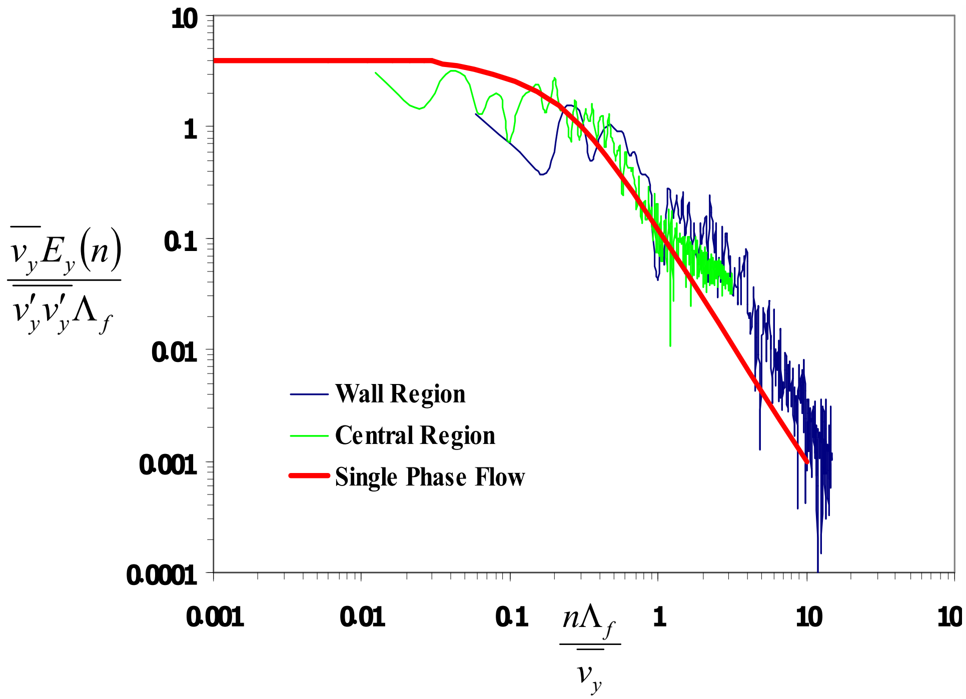


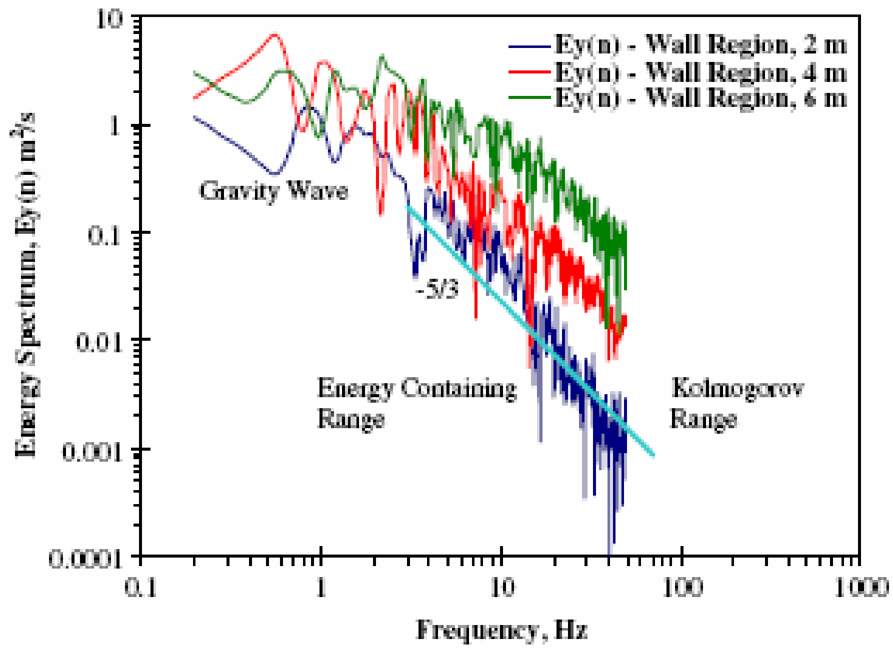


TURBULENT FLOW REGIME

Jiradilok et al. (2006), Chem. Eng. Sci. 61, 5544-5559

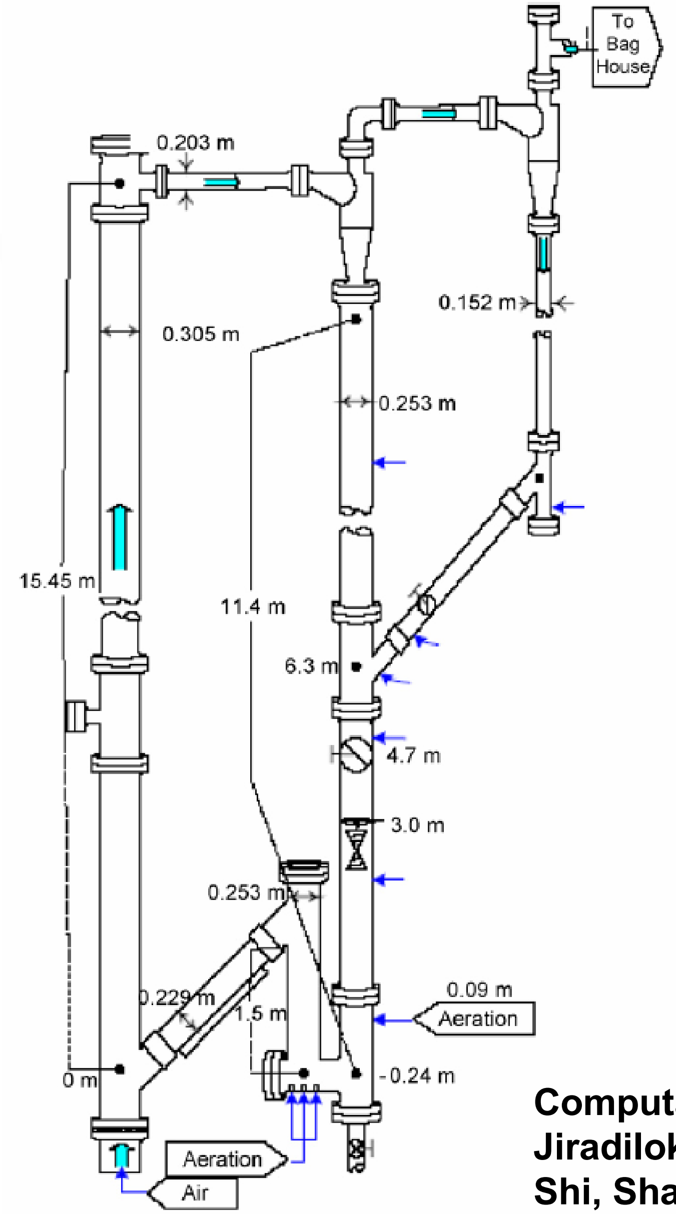
COMPUTED ENERGY SPECTRUM COMPARED TO SINGLE PHASE TURBULENT FLOW

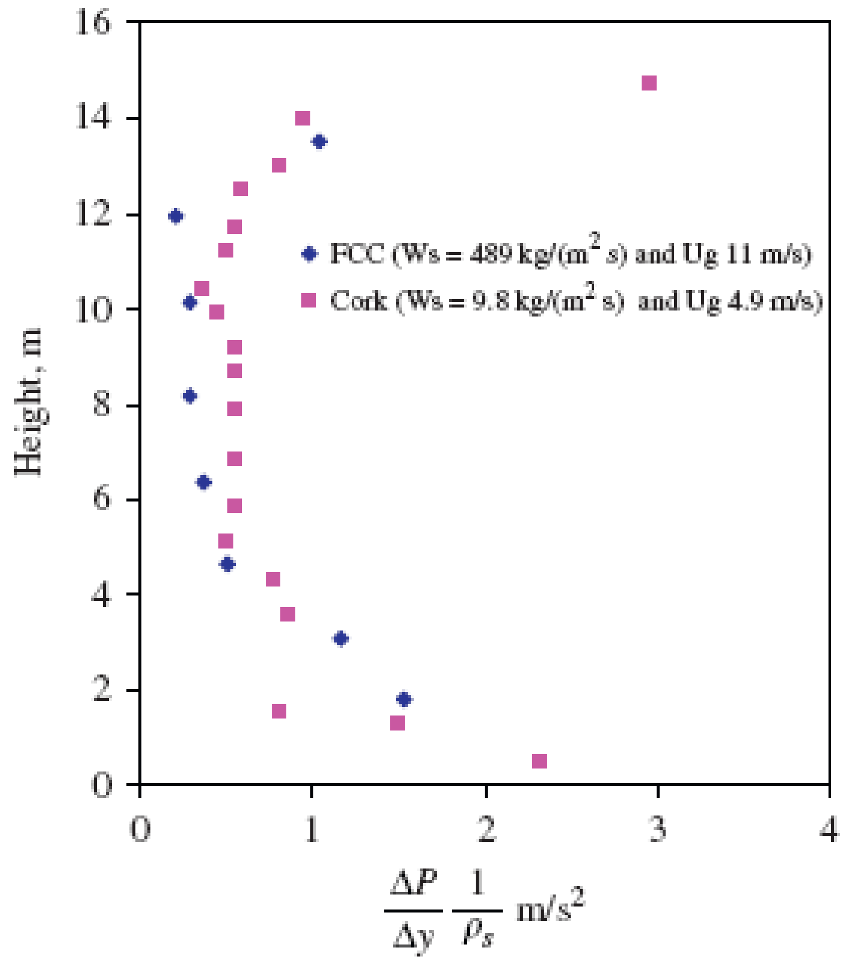




Jiradilok et al. (2006), Chem. Eng. Sci. 61, 5544-5559

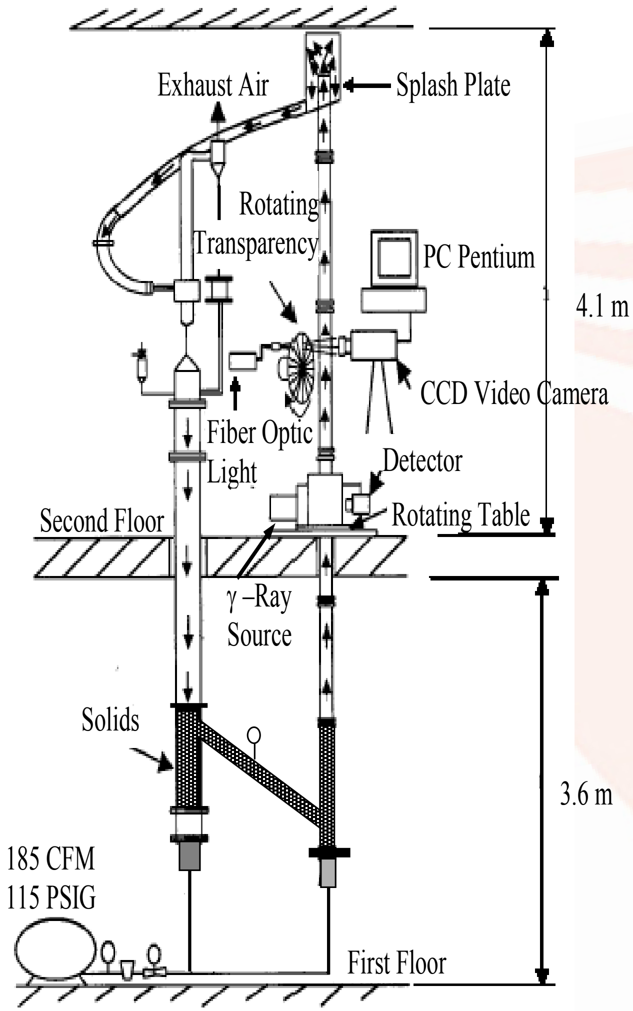
NETL AND PSRI RISERS



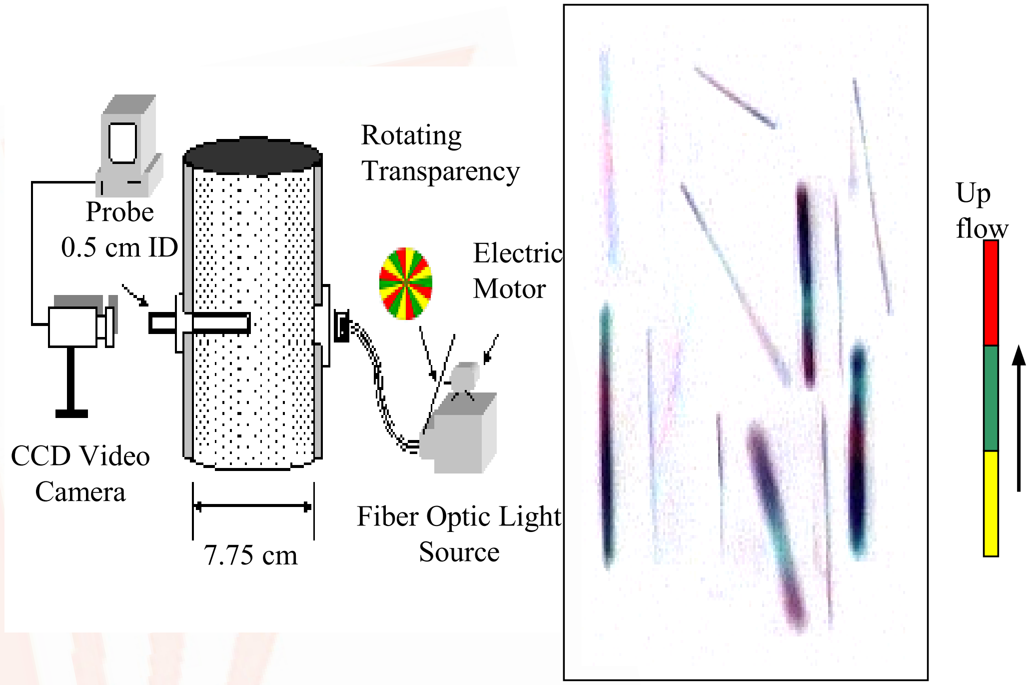


Computation of turbulence and dispersion of cork in the NETL rise, Jiradilok, V., Gidaspow, D., Breault, R.W., Shadle, L.J., Guenther, C., Shi, Shaoping, Chem. Eng. Sci. 63 (2008), 2135-2148

IIT RISER



IIT riser with splash plate and fluidized downcomer to obtain high flux



Particle image velocity measurement system with probe and typical streak images captured by the CCD camera. (Gidaspow et al. (2004))

DISPERSION COEFFICIENTS

Due to particle oscillations, "laminar"

$$D_{Particles \quad oscillations} = \frac{Granular \quad Temperature}{Friction \quad Coefficients}$$

For Brownian motion: $$D = \frac{RT}{Avagadro \quad number} \cdot \frac{1}{Friction \quad Coefficient}$$

Due to cluster or bubble, "turbulent"

$$\boxed{D_{Turbulent}(a) = \overline{v'(a)v'(a)}T_L}$$

= Turbulent Kinetic energy × Characteristic Time

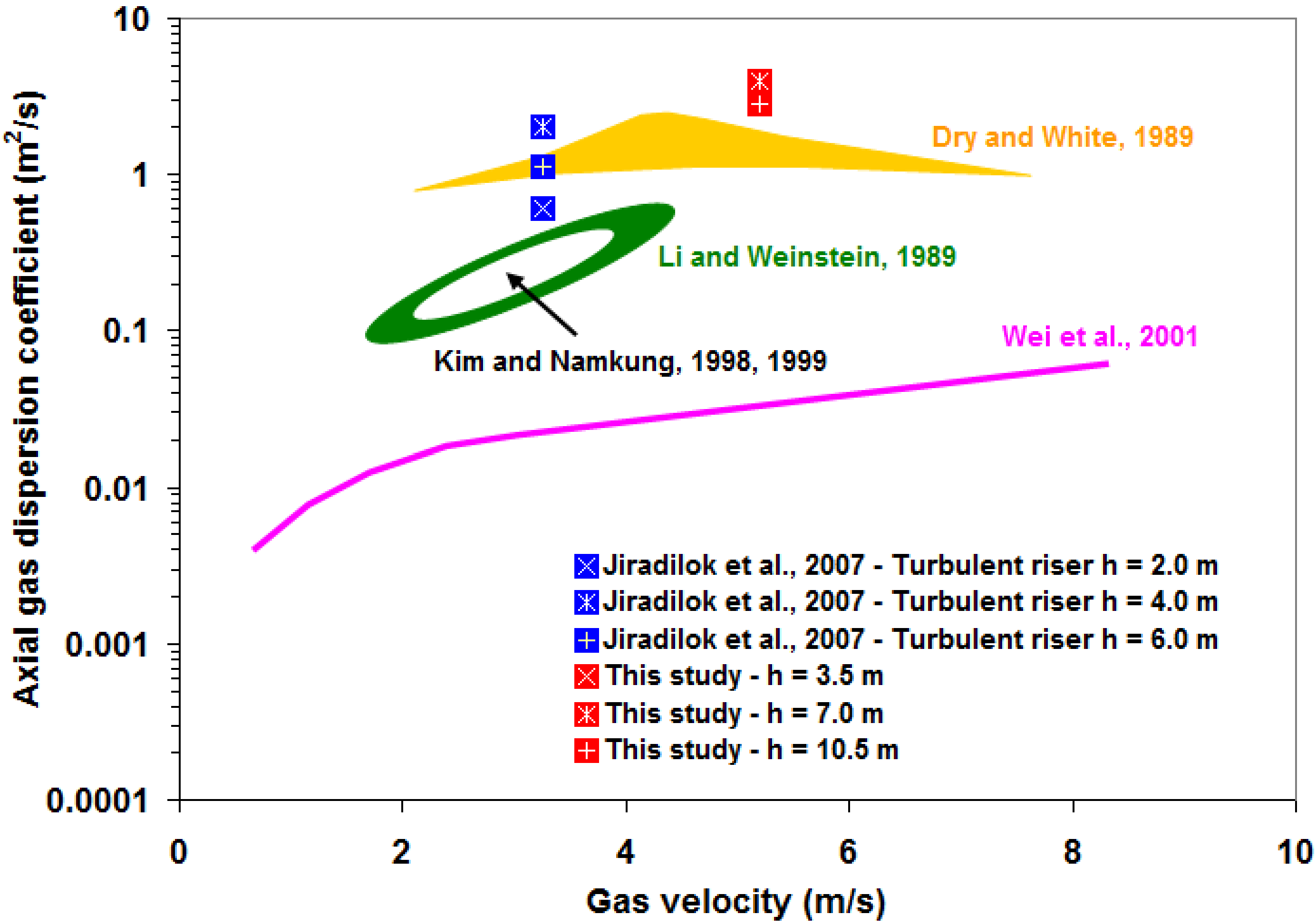
where, $\overline{v'(a)v'(a)}$ Reynolds normal stress in x or y direction

$$T_L = \int_0^\infty \frac{\overline{v'(t)v'(t+t')}}{\overline{v'^2}} dt'$$ Lagrangian integral time scale

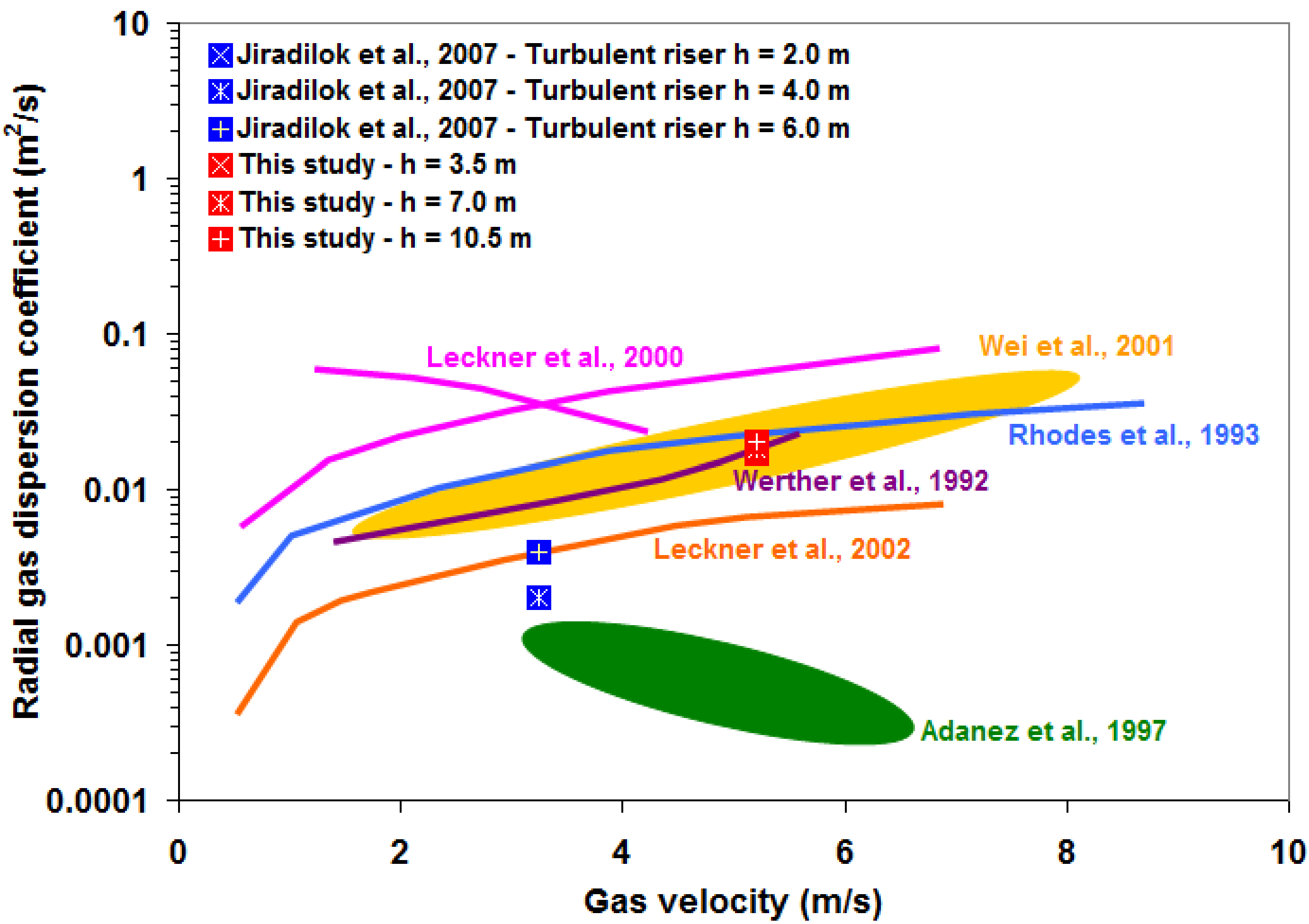
$$T_L \approx T_E$$ Eulerian integral time scale approximately equals Lagrangian integral time scale

Hinze, H. O., 1965. Turbulence. McGraw-Hill, New York.

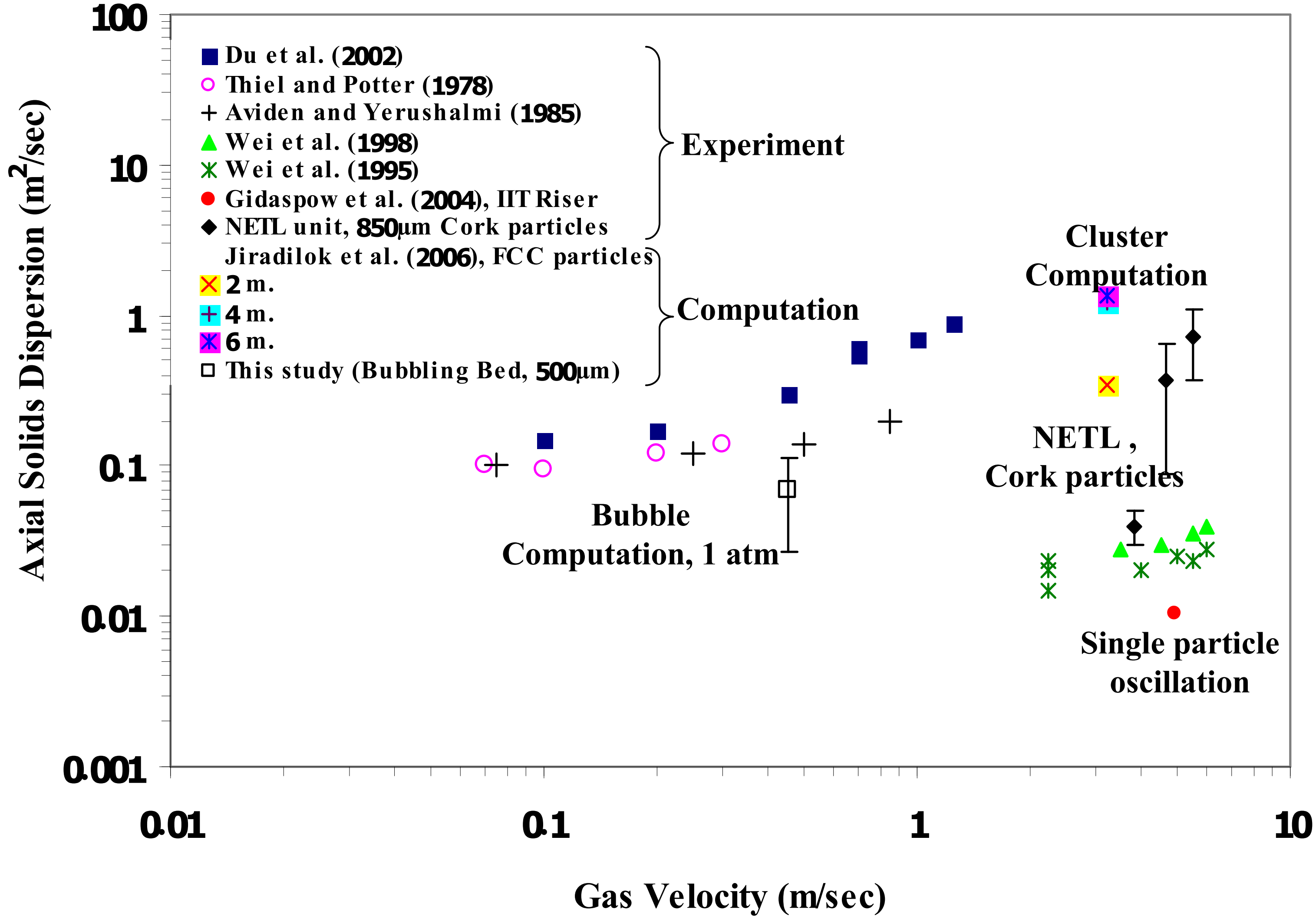
Axial Gas Dispersion Coefficients



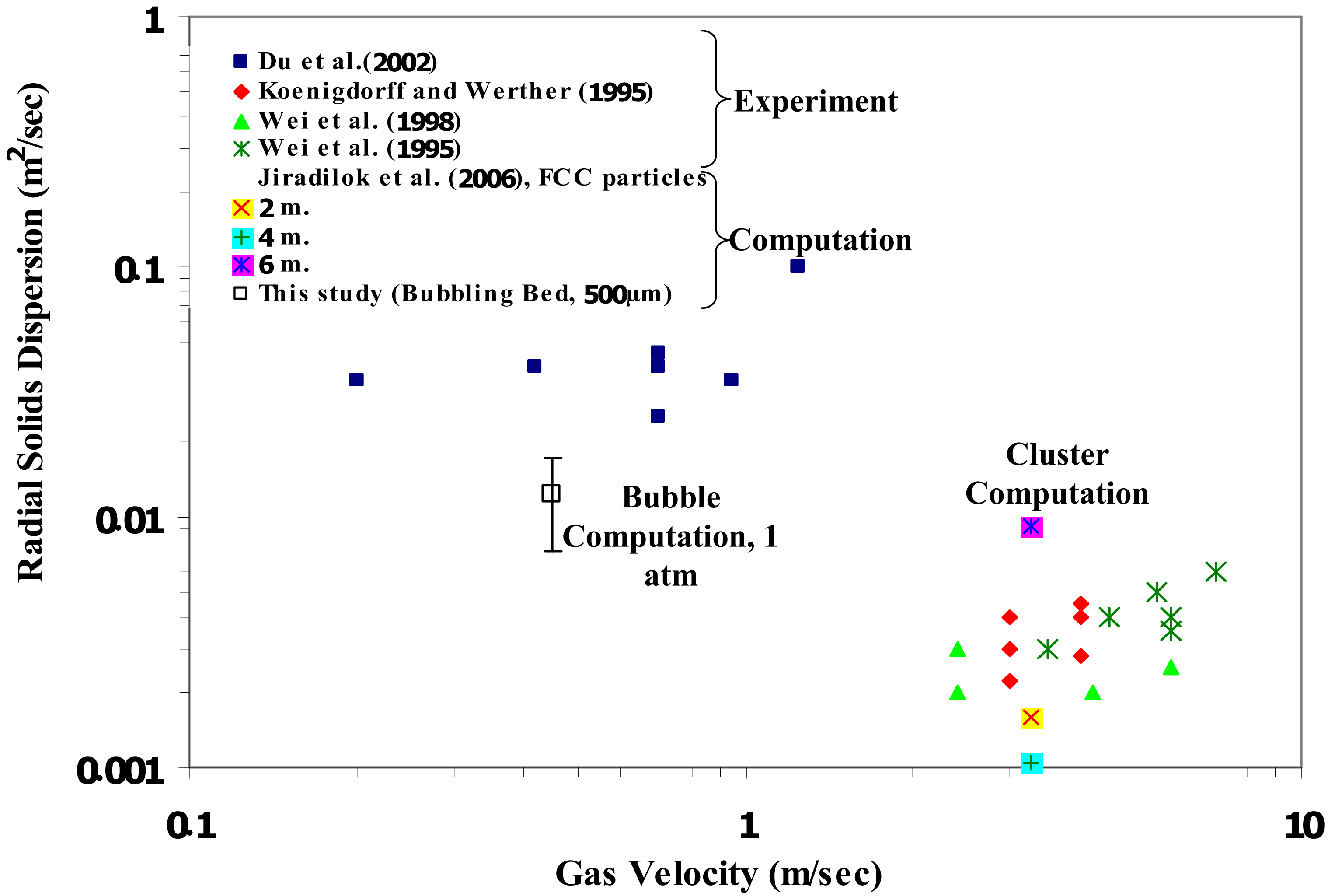
Radial Gas Dispersion Coefficients



Axial Solids Dispersion Coefficients



Radial Solids Dispersion Coefficients



IIT 2-D FLUIDIZED BED

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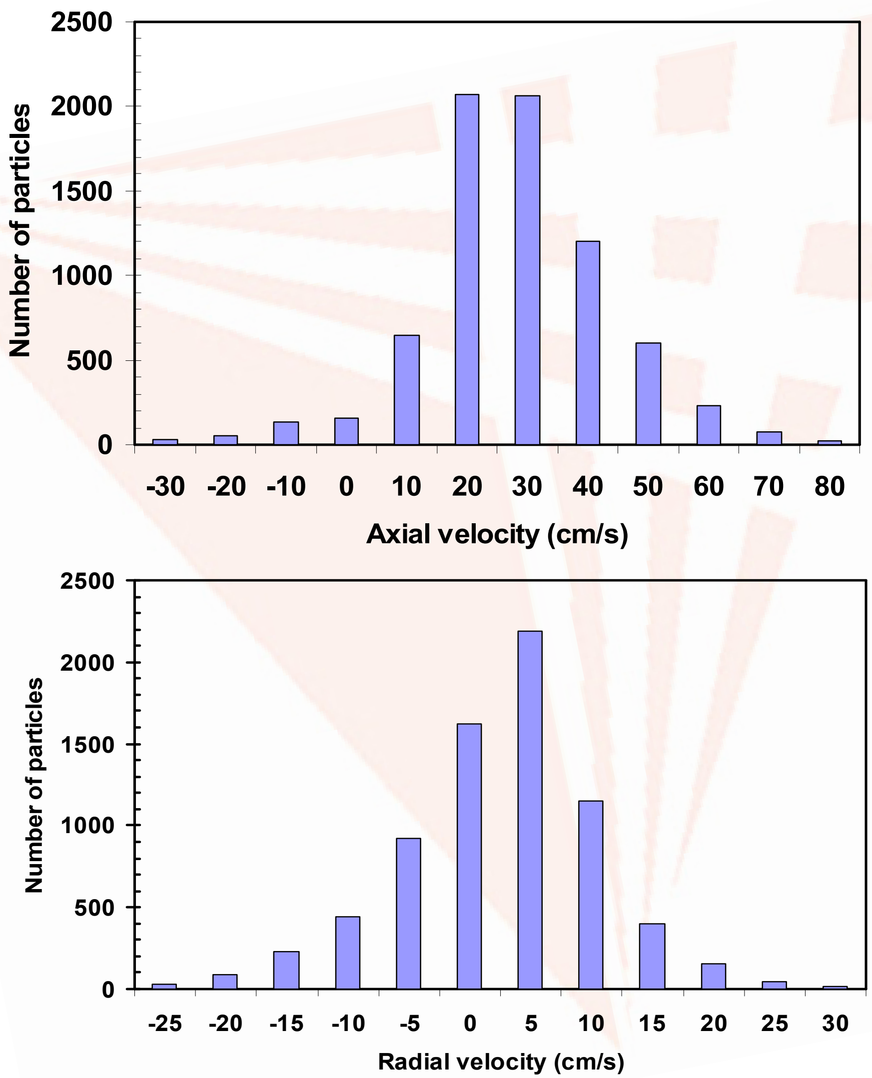
INSTANTANEOUS VELOCITES



H = 69.85 cm
U_g = 46.67 cm/s
t = 1/250 s

Comparison of laminar and turbulent granular temperatures in IIT 2- D circulating fluidized bed and IIT riser

Granular Temperature, m^2/s^2			
System	Radial Position	Laminar due to individual particle oscillations	Turbulent due to cluster oscillations
2-D CFB, 75 μm FCC particles	Center	1.27×10^{-2}	6.73×10^{-3}
2-D CFB, 75 μm FCC particles	Right Wall	6.67×10^{-3}	2.54×10^{-3}
IIT Riser, 1093 μm	Wall	9.48×10^{-2}	2.61×10^{-2}

Mixing is on the level of particles

GRANULAR TEMPERATURES

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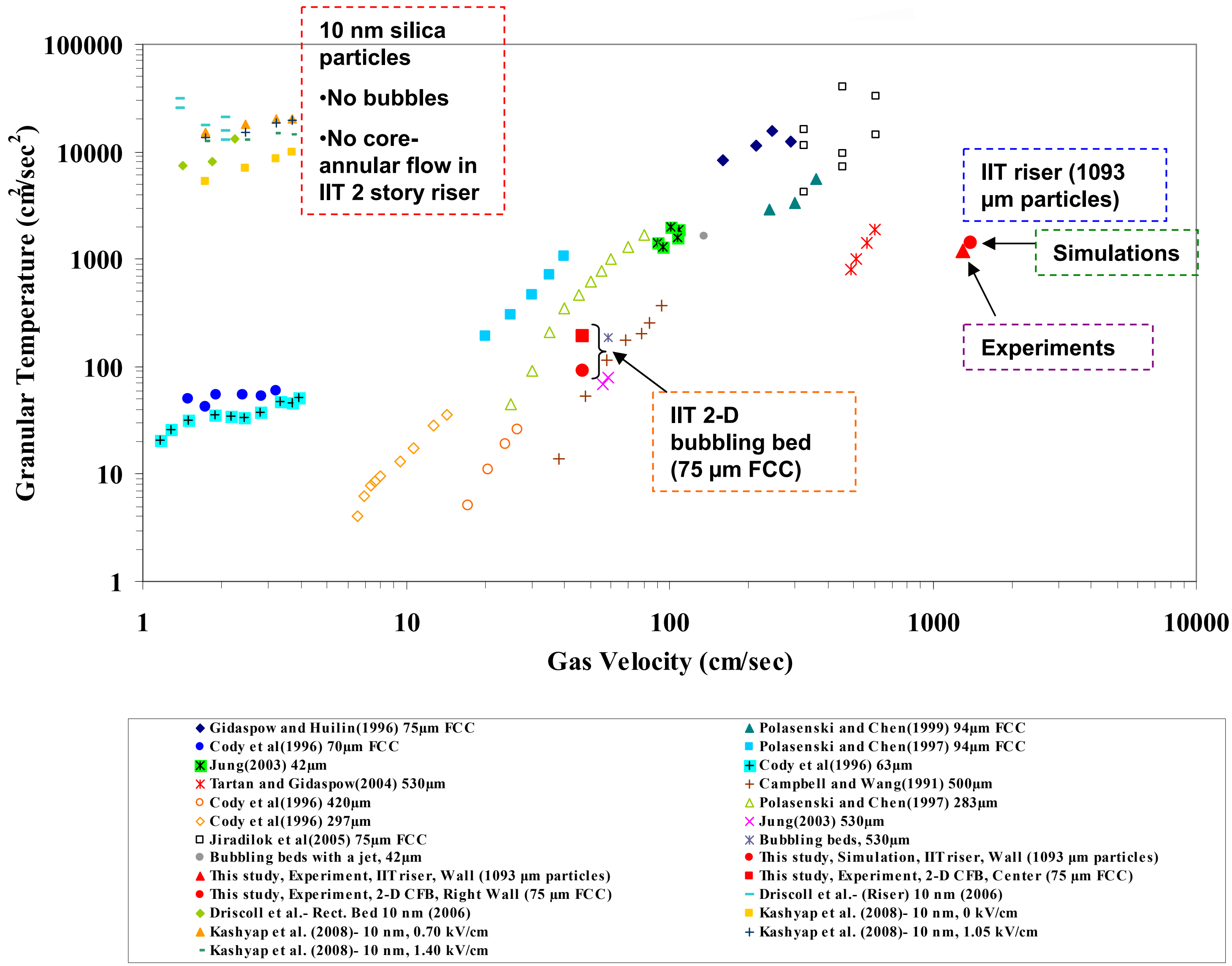

AXIAL SOLID DISPERSION COEFFICIENTS

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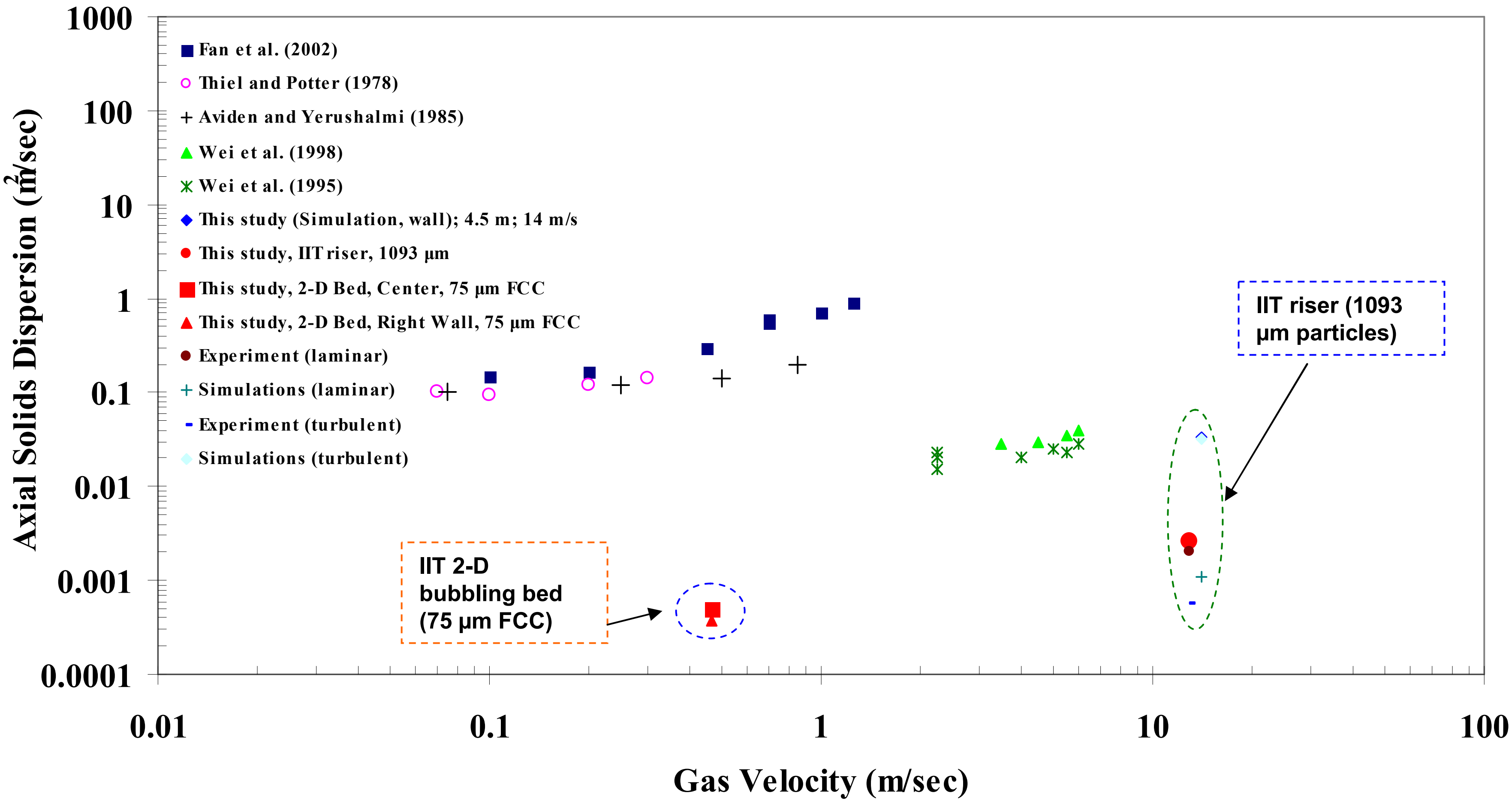

RADIAL SOLID DISPERSION COEFFICIENTS

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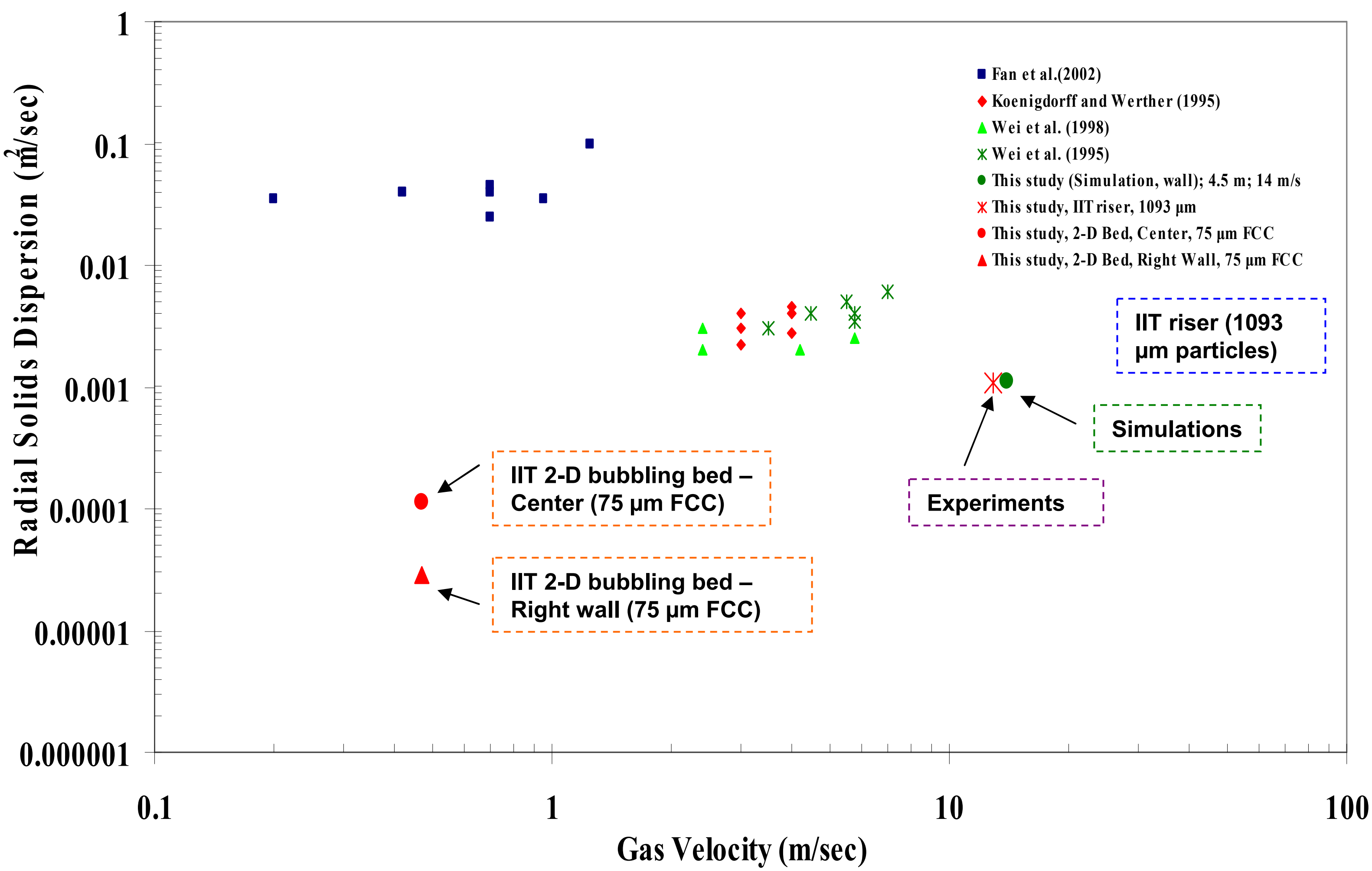

OZONE DECOMPOSITION REACTION EXPERIMENTAL SETUP

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OZONE CONCENTRATION

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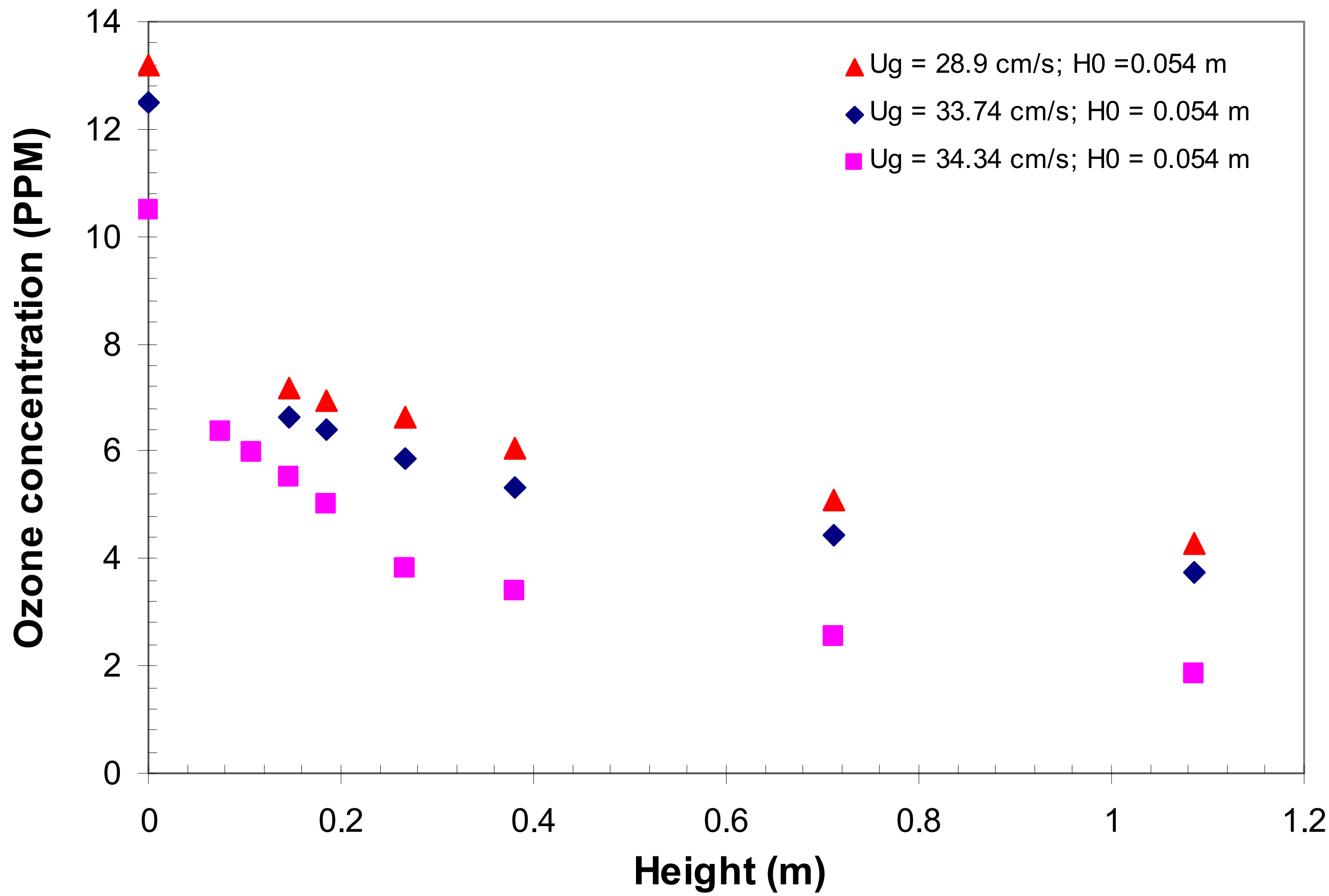


COMPUTATION OF SHERWOOD NUMBERS AND MASS TRANSFER COEFFICIENTS

Ozone decomposition reaction →

$$2O_{3(g)} \rightarrow 3O_{2(g)}$$

Conservation of species equation in the code:

$$\frac{\partial}{\partial t}(\varepsilon_g C_i) + \nabla.(\varepsilon_g C_i v_i) = k_{reaction}\varepsilon_s C_i$$

A one dimensional approximation leads to:

$$v_y \varepsilon_g \frac{dC_{O_3}}{dY} = -KC_{O_3}\varepsilon_s$$

where, "K" is the overall rate constant given by the additive resistance concept as

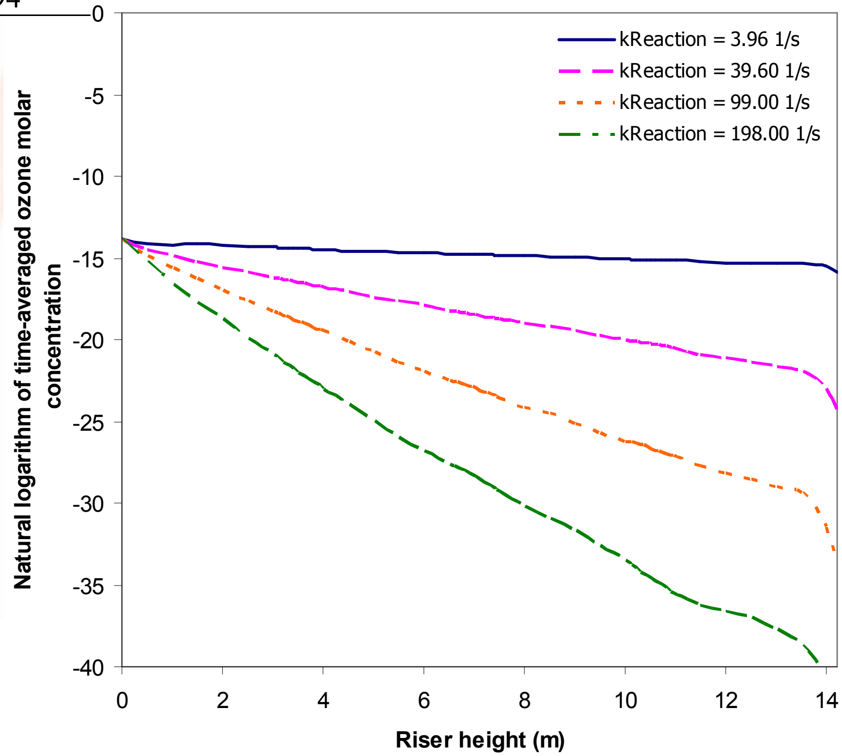
$$\frac{1}{K} = \frac{1}{k_{mass\ transfer}a_v} + \frac{1}{k_{reaction}}$$

Sherwood number,

$$Sh = \frac{k_{mass\ transfer}d_p}{D}$$

PARTICLE CLUSTER DIAMETER

Method	Height (m)	Particle cluster diameters (m)		
		Minimum	Maximum	Averaged
This study	**3.5**	0.0064	0.0232	0.0101
	7.0	0.0040	0.0238	0.0095
	10.5	0.0027	0.0150	0.0087
	Averaged	0.0027[a]	0.0238[b]	0.0095
Harris's correlation	**3.5**	0.0033	0.0151	0.0092
	7.0	0.0035	0.0149	0.0092
	10.5	0.0034	0.0165	0.0099
	Averaged	0.0033[a]	0.0165[b]	0.0095
Gu's correlation	**3.5**	0.0028	0.0154	0.0091
	7.0	0.0030	0.0149	0.0089
	10.5	0.0029	0.0175	0.0102
	Averaged	0.0028[a]	0.0175[b]	0.0094



EXAMPLE OF SHERWOOD NUMBER AND MASS TRANSFER COEFFICIENT

For PSRI riser Challenge Problem 1, overall mass transfer coefficient, *K* = 30.81 s^{-1}

(Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, "Kinetic theory based computation of PSRI riser- Part II: Computation of mass transfer coefficient with chemical reaction", Chemical Engineering Science, 64 (2009) 1212-1222)

The mass transfer coefficient is calculated from equation:

$$\frac{1}{K} = \frac{1}{k_{mass\ transfer} a_v} + \frac{1}{k_{reaction}}$$

With d_p = 76×10^{-6} m

a_v = $(3\times4\pi(\text{particle radius}^2)) / (4\pi(\text{particle radius}^3))$

= 3/particle radius

= $3/(d_p/2)$

= $3/((76\times10^{-6})/2) = 78947.37\ m^{-1}$

$k_{reaction}$ = 39.60 s^{-1}

Note that the overall resistance, 1/*K*, and the reaction resistance, $1/k_{reaction}$, are close to each other. This implies that the mass transfer resistance is small.

Therefore, $k_{mass\ transfer}\ a_v$ = 138.71 s^{-1} and

$k_{mass\ transfer}$ = 0.0018 m/s

The Sherwood number is calculated from equation:

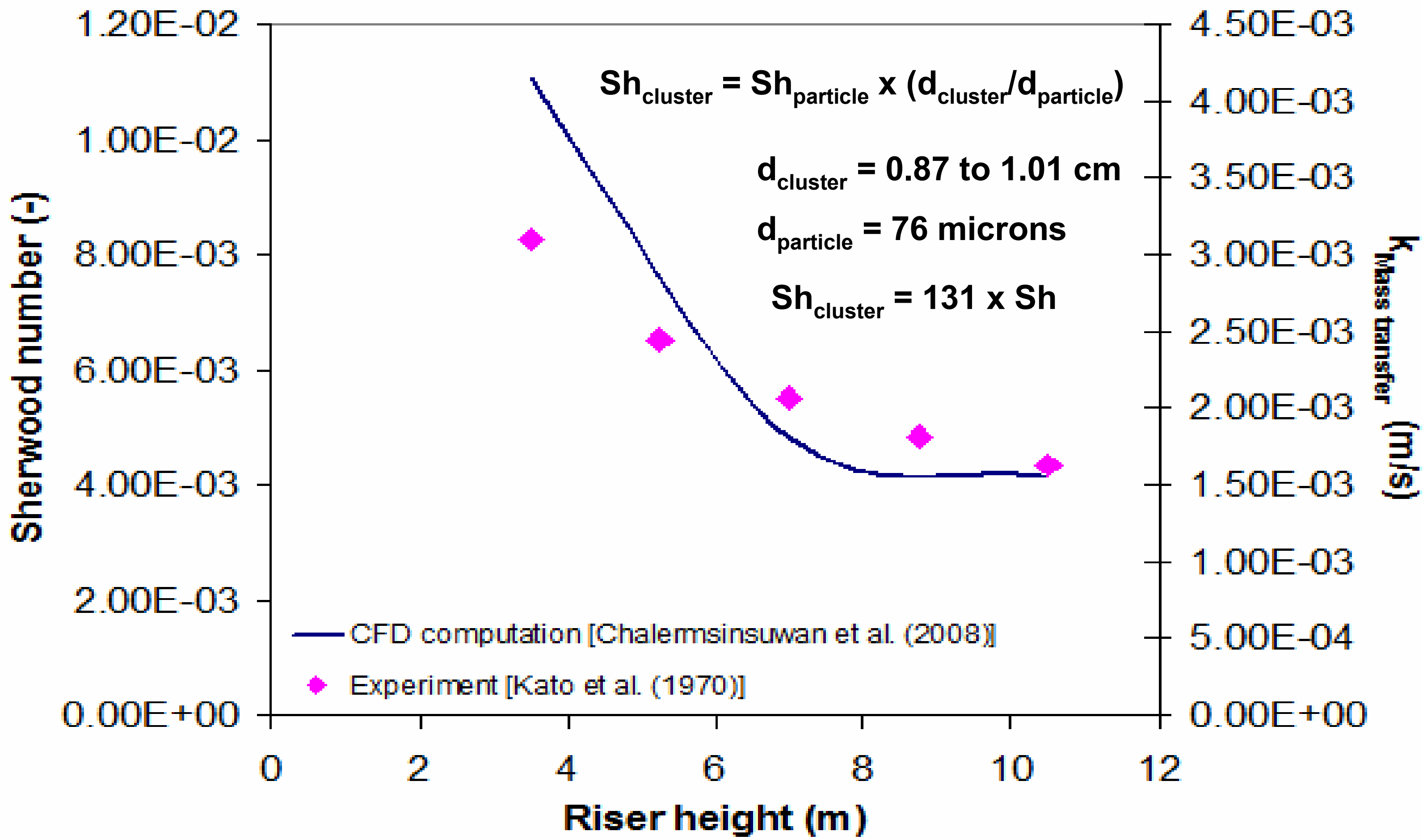
$$Sh = \frac{k_{mass\ transfer} d_p}{D}$$

With D = $2.88\times10^{-5}\ m^2/s$

Therefore, Sh = 0.0046

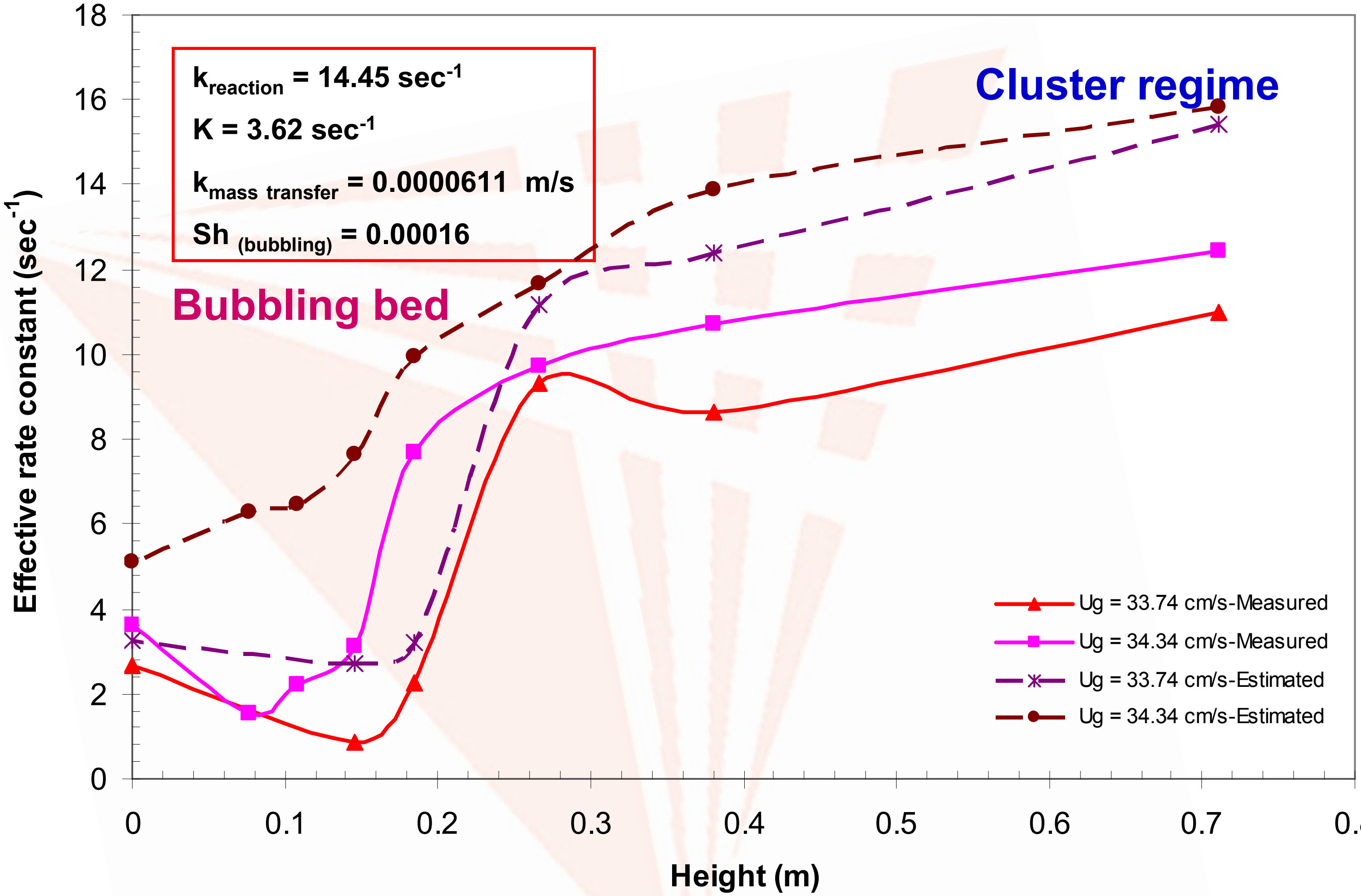
COMPUTATION OF MASS TRANSFER COEFFICIENTS

- **Example: Simulation of PSRI riser with $k_{reaction}$ = 39.6 s^{-1}**



Apparent low mass transfer coefficients in PSRI riser with $k_{reaction}$ = 39.6 s^{-1}
For Sh = 0.0111, $Sh_{cluster}$ = 1.46

EFFECTIVE RATE CONSTANT



Differential reactor analysis

$$\boxed{v_g \varepsilon_g \frac{dC}{dY} = -KC_{average}\varepsilon_s}$$

$$\boxed{U_g \frac{(C_2 - C_1)}{(Y_2 - Y_1)} = -K \frac{(C_1 + C_2)}{2} \frac{(\varepsilon_{s1} + \varepsilon_{s2})}{2}}$$

CONCLUSIONS

We have shown that the kinetic theory based CFD codes correctly compute:

(1) Dispersion coefficients

(2) Mass transfer coefficients

Hence, the kinetic theory based CFD codes can be used for fluidized bed reactor design without any such inputs

BACKUP SLIDES

FUTUREGEN: COAL GASIFIER FUEL CELL SYSTEM WITH CO_2 SEQUESTRATION

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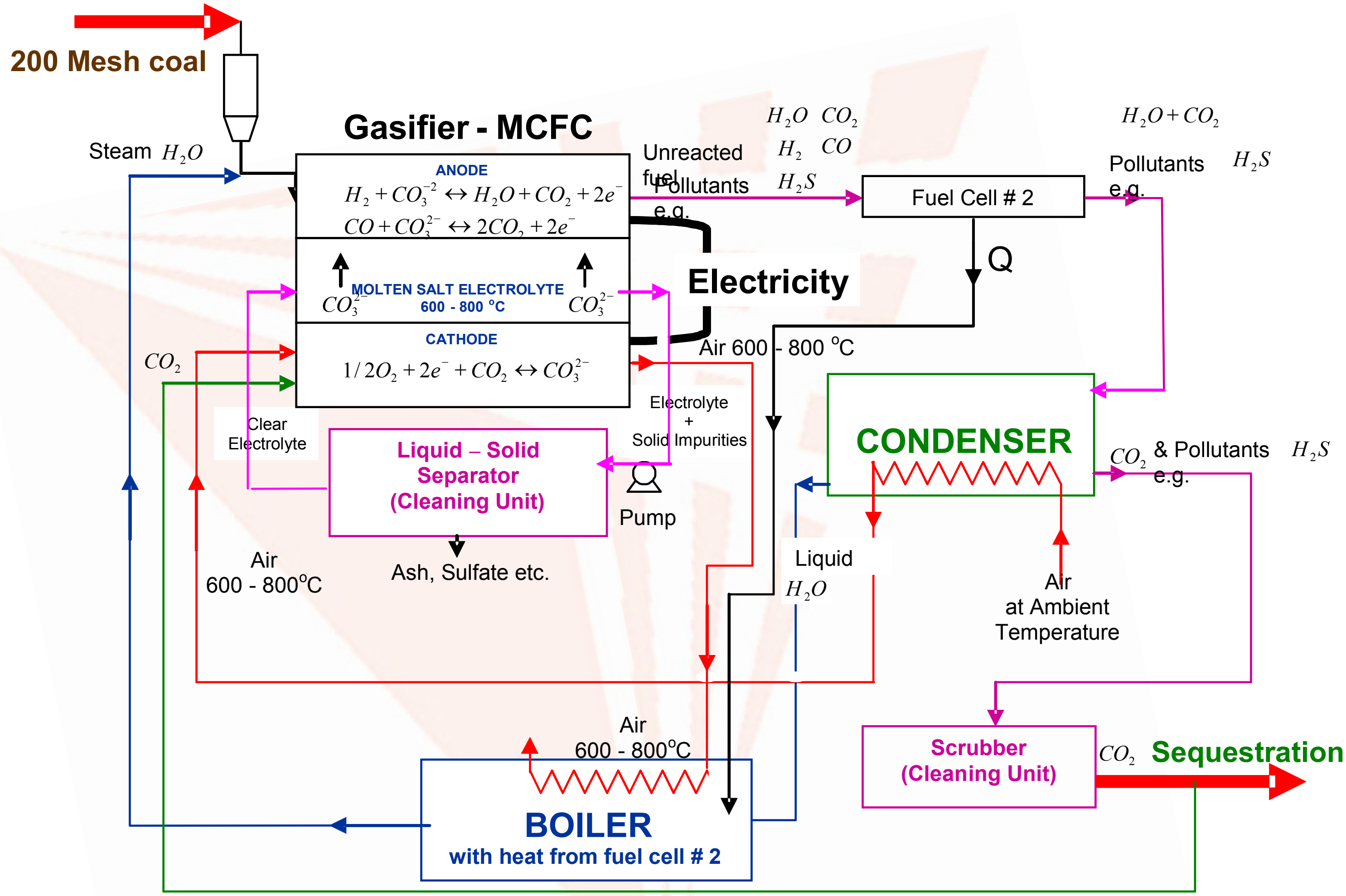

Advantages over Futuregen

- No Oxygen plant
- Water is reused
- 70% electrical efficiency

FUTUREGEN: IDEAL GASIFIER FUEL CELL WITH CARBON FEED